Equivalence of the Variational Matrix Product Method and the Density Matrix Renormalization Group applied to Spin Chains

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We present a rotationally invariant matrix product method (MPM) of isotropic spin chains. This allows us to deal with a larger number of variational MPM parameters than those considered earlier by other authors. We also show the relation between the MPM and the DMRG method of White. In our approach the eigenstates of the density matrix associated with the MPM are used as variational parameters together with the standard MPM parameters. We compute the ground state energy density and the spin correlation length of the spin 1 Heisenberg chain.

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The density matrix renormalization group (DMRG), introduced by White [1] in 1992, is a powerful numerical method to study the ground state and static properties of quantum lattice systems, as for example the Heisenberg, t-J, and Hubbard models defined on chains, ladders and clusters. The DMRG uses the Wilsonian scheme of adding one point at each RG step. After many iterations the DMRG reaches a fixed point, and the ground state exhibits a matrix product structure (MP), as was shown by Ostlund and Rommer [2]. These authors proposed to start from a MP ansatz for the ground state of the system, determining the variational parameters by the standard variational method, without resorting to the DMRG. The advantage of the MPM is that it is analytical and does not require big computational resources. However it is not clear how to treat large values of the number of states m used in the minimization of the energy. On the other hand it is not clear the relation between the MPM and the DMRG, apart from sharing a MP structure in the thermodynamic limit.

In this letter we show i) how to treat numerically and analytically larger values of m than those considered by other authors, thanks to the reduction of the basis obtained by exploiting the rotational symmetry of the problem and ii) exhibit the relation between the MPM and the DMRG. In particular we shall see that the MPM naturally leads to a density matrix whose eigenvalues appear as variational parameters together with those that generate the MP ansatz. In fact our formalism is closely connected to that developed in ref [3] (see also [4,5]). We apply the MPM and the DMRG to the spin 1 Heisenberg chain, and compare the results obtained with both methods. For the ground state energy density, the MPM gives a better estimate for all values of $m > 1$, which we interpret as been caused by the existence of a bound state in the middle of the superblock in the DMRG method. In the MPM this bound state is absent by construction. For increasing values of m the discrepancy between the MPM and the DMRG tends to disappear. The numerical results for the eigenvalues of the density matrices in both methods are similar, and they seem to converge to a common value when increasing m. From these results we conclude the equivalence between the MPM and the DMRG methods in the thermodynamic limit for large values of m.

We shall consider a spin chain with spin S at each site, where S is an integer (the case of half integer spin will be treated in a separate work). Let us denote the basis states of the MPM as $|a, JM\rangle_N$, where N is the length of the chain, $a = 1, \cdots, d_J$ denotes the multiplicity of the total spin J of the state and M is the third component of the spin. Counting the number of multiplets we have $m = \sum_J \; d_J$, which correspond to a number $m_W = \sum_J (2J+1)\, d_J$ of states in the standard DMRG. At the fixed point of the DMRG one has the matrix product law [2],

$$|a_1, J_1 M_1\rangle_N = \sum_{a_2 J_2, M_2, M} \; A_{a_1 J_1, a_2 J_2} \tag{1}$$

$$\times \, |SM\rangle_N \; \otimes |a_2, J_2 M_2\rangle_{N-1} \; \langle SM, J_2 M_2 \, | J_1 M_1 \rangle$$

where $\langle SM, J_2 M_2 \, | J_1, M_1 \rangle$ are Clebsch-Gordan coefficients and $A_{a_1 J_1, a_2 J_2}$ are variational parameters subject to the following conditions

$$A_{a_1 J_1, a_2 J_2} = 0 \;\; \text{unless} \;\; |J_2 - S| \leq J_1 \leq J_2 + S \tag{2}$$

$$\sum_{a_2, J_2} A^*_{a_1 J_1, a_2 J_2} \; A_{a'_1 J_1, a_2 J_2} = \delta_{a_1 a'_1} \tag{3}$$

Eq.(2) follows from the CG decomposition $S \otimes J_2 \rightarrow J_1$ in (1), while condition (3) guarantees that the states $|a, JM\rangle_N$ constitute an orthonormal basis for all values of N. The initial data of the recurrence relation (1) is given by choosing a spin $S/2$ irrep at the end of the chain. This choice eliminates the multiplicity associated to the effective spins $S/2$ at the ends of the chain. The sum

in $J's$ in eq. (1) is of course restricted to a finite set of spins.

The parameters $A_{a_1 J_1, a_2 J_2}$ are determined by minimizing the energy of the states $|a, JM\rangle_N$ in the limit where $N \to \infty$. For this purpose let us define the following quantity,

$$E^{(N)}_{aa'J} =_N \langle a, JM| H_N |a', JM\rangle_N \tag{4}$$

where H_N is the Hamiltonian acting on the chain with N sites. From eq.(1) one can derive a recursion formula for $E^{(N)}_{aa'J}$,

$$E^{(N)}_{aa'J} = V_{aa'J} + \sum_{bb'J'} T_{aa'J,bb'J'}\ E^{(N-1)}_{bb'J'}, \quad (N \geq 3) \tag{5}$$

where $\mathbf{T}$ is a matrix with entries (we assume from now on the reality of $A_{a_1 J_1, a_2 J_2}$),

$$T_{aa'J,bb'J'} = A_{aJ,bJ'}\ A_{a'J,b'J'} \tag{6}$$

and W is the matrix element of the piece of the Hamiltonian which couples the sites N and $N-1$, which does not dependent on N,

$$V_{aa'J} =_N \langle a, JM| H_{N-1,N} |a', JM\rangle_N \tag{7}$$

For the Heisenberg model, $H_{N-1,N} = \mathbf{S}_{N-1} \cdot \mathbf{S}_N$, and applying the Wigner-Eckart theorem, we find the following expression for W in terms of 6-j symbols,

$$\begin{aligned} V_{a_1 a_2 J_1} = \textstyle\sum_{a_3 J_2, a_4 J_3, a_5 J_4}\ \mathcal{H}_{J_1 J_2 J_3 J_4} \\ A_{a_1 J_1, a_3 J_2} A_{a_2 J_1, a_4 J_3}\ A_{a_3 J_2, a_5 J_4} A_{a_4 J_3, a_5 J_4}, \end{aligned} \tag{8}$$

$$\begin{aligned} \mathcal{H}_{J_1,J_2,J_3,J_4} = (-)^{2S+J_1+J_2+J_3+J_4+1}\, S\,(S+1)\,(2S+1) \\ \times \sqrt{(2J_2+1)\,(2J_3+1)} \begin{Bmatrix} 1 & S & S \\ J_1 & J_2 & J_3 \end{Bmatrix} \begin{Bmatrix} 1 & S & S \\ J_4 & J_2 & J_3 \end{Bmatrix} \end{aligned} \tag{9}$$

The solution of (5) can be expressed in matrix notation as,

$$|E^{(N)}\rangle = \left(1 + \mathbf{T} + \mathbf{T}^2 + \ldots + \mathbf{T}^{N-3}\right)\ |W\rangle + \mathbf{T}^{N-2}\ |E^{(2)}\rangle \tag{10}$$

where $|E^{(N)}\rangle$ is regarded in (10) as a vector whose components are labeled by $(aa'J)$. The entries of $\mathbf{T}$ are given by eq.(6).

In the limit $N \to \infty$ the contribution from $|E^{(2)}\rangle$ drops off and we shall show below that $E^{(N)}_{aa'J}$ behaves as,

$$\lim_{N\to\infty} \frac{1}{N}\ E^{(N)}_{aa'J} = \ \delta_{aa'}\ \ e_\infty \tag{11}$$

where e_∞ can be identified with the ground state energy density and it reads,

$$e_\infty = \sum_{aa'J}\ \rho_{aa'J}\ V_{aa'J} \tag{12}$$

In eq.(12) $\rho_{aa'J}$ is the right eigenvector of the matrix $\mathbf{T}$ with eigenvalue 1, and plays the role of a density matrix in the MPM. The proof of eqs.(11) and (12) follows from the existence of an eigenvalue of the matrix $\mathbf{T}$ equal to 1 [3,2]. This property can be deduced from the normalization condition (3). Let us call $|v\rangle$ and $\langle\rho|$ the right and left eigenvectors associated to the eigenvalue 1 of $\mathbf{T}$, which we shall assume to be unique,

$$\mathbf{T}\ |v\rangle = |v\rangle \tag{13}$$

$$\langle\rho|\ \mathbf{T} = \langle\rho| \tag{14}$$

Then eq. (3) implies that $|v\rangle$ is given in components by $v_{aa'J} = \delta_{aa'}$.. On the other hand the quantities $\rho_{aa'J}$ that appear in (12) are nothing but the components of $\langle\rho|$, and they are found by solving the eigenvalue problem (14). In eq.(12) we have normalized $\langle\rho|$ according to,

$$\langle\rho|v\rangle = 1\ \to\ \sum_{aa'J}\ \rho_{aa'J} = 1 \tag{15}$$

In a field theoretical language $|v\rangle$ and $\langle\rho|$ play the role respectively of incoming $|0\rangle$ and outgoing vacua $\langle 0|$, which are left invariant by the transfer matrix operator $\mathbf{T}$, that shifts by one lattice space the spin chain. On the other hand $\rho_{aa'J}$, has the properties of a density matrix, and it corresponds precisely to the reduced density matrix of the blocks in the DMRG formalism, as we shall show below. It is remarkable that the MP ansatz (1) leads in a natural way to a density matrix formalism. This suggest that a rigorous mathematical formulation of the DMRG could perhaps be achieved within the MPM.

By analogy with the DMRG we may choose a basis where the density matrix becomes diagonal, i.e. $\rho_{aa'J} = w^2_{aJ}\ \delta_{aa'}$. Under this assumption eq.(14) reads,

$$\sum_{a_1 J_1}\ w^2_{a_1 J_1}\ A_{a_1 J_1, a_2 J_2}\ A_{a_1 J_1, a'_2 J_2} = \ w^2_{a_2 J_2}\ \delta_{a_2 a'_2} \tag{16}$$

A solution of eqs.(16) is obtained using eq.(3) and assuming the following "detailed balanced" condition [9],

$$w_{a_1 J_1}\ A_{a_1 J_1, a_2 J_2}\ \ = \ w_{a_2 J_2}\ A_{a_2 J_2, a_1 J_1} \tag{17}$$

This eq. is very useful since we can eliminate almost a half of the $A's$ in terms of the other half, and use the $w's$ as independent variationally parameters. Hence the problem reduces to the minimization of the GS energy (12) with respect to the variational parameters w_{aJ} and $A_{a_1 J_1, a_2 J_2}$ subject to the constraints (2),(3) and (17). For a MP ansatz with no multiplicities, i.e. $d_J = 1$, one can solve all the constraints in terms of an independent set of parameters, however when $d_J > 1$ it is more efficient to use a numerical program of minimization with constraints.

Taking into account all the variables and constraints one sees that the total number of independent variational parameters, N_A, is given by,

$$N_A = \frac{1}{2} \sum_{J_1 \neq J_2} \Lambda_{J_1 J_2} \; d_{J_1} \, d_{J_2} \; + \sum_J \, d_J - 1 \qquad (18)$$

where $\Lambda_{J_1 J_2}$ is 1 if J_1 and J_2 satisfy eq.(2) and zero otherwise.

In table 1 we present the results for the case of spin $S = 1$, obtained with the MPM and a version of the DMRG where the rotational symmetry has been used to eliminate the redundancy in the states kept [6]. The case $m = 1$ corresponds to the AKLT wave function [7,8], where e_∞ computed with the MPM and the DMRG coincide. This is because from eq.(18) there is no adjustable parameter in the ansatz. The case $m = 4$ is the one considered in [2]. The ground state energy $e_\infty(m)$ obtained with the MPM is always lower than DMRG energy, this is related to the fact that the wave function generated by the infinite system DMRG is not uniform. The DMRG optimizes the ground state of the renormalized system $[B] \bullet \bullet [B]$, where $[B]$ denotes the m-state block spin, while the super block $[B \bullet]$ has $3m$ degrees of freedom. From the view point of the MPM, the super block $[B \bullet]$ should be optimized with m degrees of freedom. As a result, a shallow bound-state appears between left-half of the system $[B] \bullet$ and the right half $\bullet [B]$, and the numerical precision in the ground state energy is spoiled in DMRG, especially when m is small. A way to improve the DMRG from this error is to consider a system $[B] \bullet [B]$ at the last several steps in the infinite/finite system DMRG algorithm. By choosing the block configuration, the degree of freedom of the superblock $[B \bullet]$ is automatically restricted to m because the 'reservoir' $[B]$ has only m degrees of freedom.

In order to compute the spin-spin correlation lengths ξ of the MP states (1), we have to find out a recursion formula for the reduced matrix elements of the spin operators $\mathbf{S}$, which is given by

$$\begin{aligned} &{}_N\langle a_1 J_1 || \mathbf{S}_1 || a_2 J_2 \rangle_N \qquad (19) \\ &= \textstyle\sum_{a_3 J_3 a_4 J_4} \; T^{(1)}_{a_1 J_1 a_2 J_2, a_3 J_3 a_4 J_4} \; {}_{N-1}\langle a_3 J_3 || \mathbf{S}_1 || a_4 J_4 \rangle_{N-1} \end{aligned}$$

with

$$\begin{aligned} T^{(1)}_{a_1 J_1 a_2 J_2, a_3 J_3 a_4 J_4} &= (-)^{J_2 + J_3 + S + 1} \; A_{a_1 J_1, a_3 J_3} A_{a_2 J_2, a_4 J_4} \qquad (20) \\ &\times \sqrt{(2J_1 + 1)\,(2J_2 + 1)} \; \left\{ \begin{array}{ccc} J_3 & J_1 & S \\ J_2 & J_4 & 1 \end{array} \right\} \end{aligned}$$

The correlation length ξ is then given by the highest eigenvalue λ, in absolute value, of $\mathbf{T^{(1)}}$ by the formula,

$$\xi = -1/\ln\lambda \qquad (21)$$

For the AKLT case (i.e. $d_J = \delta_{J,1/2}$), eqs.(19) and (20) reproduce the exact spin-spin correlator found in ref. [8]. To analyze in more detail the relation MPM versus DMRG we give in table 2 the eigenvalues of the matrix $\rho_{aa'J}$, and those of the DMRG reduced density matrix in the case where $m = 6$. The later matrix has dimension $3m$ and the truncation DMRG method consists in choosing m states with highest eigenvalues $w^2_{\rm DMRG}$, which add up to $1 - P_m$ (see table 1). For this reason we have to scale the DMRG weights of the states kept in order that they sum up to 1.

$$\overline{w}^2_{\rm DMRG} = w^2_{\rm DMRG} / P_m \qquad (22)$$

In summary the results shown in tables 1 and 2 suggest that the predictions made by the MPM and the DMRG should become identical for large values of m. In a later publication we shall present the results for the spin gap and other observables for various spin chains and ladders using the MPM. An interesting problem is the generalization of the MPM to the case of holes. The results of reference [11] concerning the tJ ladder suggest that this generalization is possible and worthwhile studying it.

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m	N_A	$d_{1/2}$	$d_{3/2}$	$d_{5/2}$	$-e_\infty^{\rm MP}$	$-e_\infty^{\rm DMRG}$	$1-P_m$	$\xi^{\rm MP}$
1	0	1	0	0	1.333333	1.333333	1.6×10^{-2}	0.910
2	2	1	1	0	1.399659	1.369077	1.4×10^{-3}	2.600
3	4	2	1	0	1.401093	1.392515	1.3×10^{-5}	3.338
4	7	2	2	0	1.401380	1.401380	1.6×10^{-5}	3.937
5	10	2	2	1	1.401443	1.401436	7.6×10^{-6}	4.085
6	13	2	3	1	1.401474	1.401468	1.3×10^{-6}	4.453

Table 1. m is total the number of multiplets, N_A is the number of independent variational parameters, d_J is the number of multiplets with spin J, $e_\infty^{\rm MP,DMRG}$ is the GS energy density of the MPM (DMRG), $1-P_m$ is the probability of the states truncated out in the DMRG and $\xi^{\rm MP}$ is the spin correlation length of the MP state. The exact results are given by $e_\infty = 1.4014845$ and $\xi = 6.03$ [10].

a	J	w^2_{MP}	$\overline{w}^2_{DMRG}$
1	1/2	.9695581	.9696232
2	1/2	.0007662	.0007599
1	3/2	.0295443	.0294877
2	3/2	.0001119	.0001089
3	3/2	.0000078	.0000085
1	5/2	.0000118	.0000118

Table 2. a and J are the labels of the irrep, w^2_{MP}, are the eigenvalues of the MP density matrix, and $\overline{w}^2_{DMRG}$ are the corresponding DMRG eigenvalues kept in the RG process and normalized to 1. The data correspond to $m = 6$.

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